Isopropyl ether

108-20-3 | DTXSID4021890

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.00

Global applicability domain: Inside

Local applicability domain index: 6.07e-01

Confidence level: 6.04e-01

Nearest Neighbors from the Training Set

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N-Methylaniline
Measured: 10.0
Predicted: 5.88

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Quinoline
Measured: 3.80
Predicted: 6.66

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4-Vinylpyridine
Measured: 72.4
Predicted: 5.63

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Methyl tert-butyl ether
Measured: 1.51
Predicted: 3.67

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N,N-Dimethylaniline
Measured: 7.94
Predicted: 5.84